WHAT IS CLAIMED IS:

1.   A method of computer modeling the behavior of a molecule or set of molecules, comprising

selecting a model for said molecules, said model having equations of motion for said molecule;

formulating said equations of motion in Residual Form; and

integrating said model equations with an implicit integrator;

whereby computer calculations for said molecular behavior are reduced.

2.   The method of claim 1 wherein said equations of motion in Residual Form comprise

$$\begin{pmatrix} \rho_q \\ \rho_u \end{pmatrix} = \begin{pmatrix} \dot{q} - W(q)u \\ M(q)\ddot{u} - f(t,q,u) \end{pmatrix}$$

where q represents generalized system coordinates, u represents generalized velocities, W represents a generalized joint map matrix, M represents generalized system mass, f represents generalized system forces, and t represents time.

3.   The method of claim 2 wherein said integrating step is performed iteratively and residuals $\begin{pmatrix} \rho_q \\ \rho_u \end{pmatrix}$ are reduced below predetermined amounts before a next iterative integration step is performed.

4.   The method of claim 1 wherein said model comprises

a plurality of rigid bodies, each rigid body representing a portion of said molecule; and

a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies.

5.   The method of claim 4 wherein each hinge connection comprise a connection selected from the group comprises a slider joint, a pin joint, a ball joint, a free connection, and combinations thereof.

6.   The method of claim 5 wherein q correspond to internal coordinates of one of said rigid bodies with respect to another of said rigid bodies.

7.   The method of claim 6 wherein said internal coordinates comprise a linear displacement of said one rigid body with respect to said another rigid body.

8.   The method of claim 6 wherein said internal coordinates comprise an angular displacement of said one rigid body with respect to said another rigid body.

9.   The method of claim 6 wherein said internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body.

10.   The method of claim 6 wherein M comprises a system mass matrix.

11.   The method of claim 6 wherein f comprises a bias-free hinge torque.

12.   The method of claim 1 wherein said implicit integrator comprises an L-stable integrator.

13.   The method of claim 12 wherein said L-stable integrator comprises an integrator from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4 and other implicit Runge-Kutta methods.

14.   A method of claim 1 wherein said implicit integrator comprises an integrator from the group comprising DASSL and other implicit multistep methods for ODE or DAE systems.

15.   A method of computer modeling the behavior of a molecule, said molecule having a plurality of bodies having masses, said method comprising

selecting a model for said molecule, said model having equations of motion for said molecule;

formulating said equations of motion such that mass matrices corresponding to said masses for said plurality of bodies are not inverted; and

integrating said model equations with an implicit integrator; whereby computer calculations for said molecular behavior are reduced.

16.   The method of claim 15 wherein said equations of motion are in Residual Form.

17.   The method of claim 15 wherein said implicit integrator comprises an L-stable integrator.

18.   The method of claim 17 wherein said L-stable integrator comprises an integrator from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4 and other implicit Runge-Kutta methods.

19.   A method of claim 15 wherein said implicit integrator comprises an integrator from the group comprising DASSL and other implicit multistep methods for ODE or DAE systems.

20.   Computer code for modeling the behavior of a molecule, said code comprising

a model for said molecule, said model having equations of motion for said molecule, said equations of motion formulated in Residual Form; and

an implicit integrator for integrating said model equations over time;

whereby computer calculations from said code to model said molecular behavior are reduced.

21.   The computer code of claim 20 wherein said equations of motion in Residual Form comprise

$$\begin{pmatrix} \rho_q \\ \rho_u \end{pmatrix} = \begin{pmatrix} \dot{q} - W(q)u \\ M(q)\dot{u} - f(t,q,u) \end{pmatrix}$$

where q represents generalized system coordinates, u represents generalized velocities, W represents a generalized joint map matrix, M represents generalized system mass, f represents generalized system forces.

22.   The computer code of claim 21 wherein said implicit integrator integrates said model equations iteratively, and after residuals $\begin{pmatrix} \rho_q \\ \rho_u \end{pmatrix}$ are reduced below predetermined amounts before a next iterative integration is performed.

23.   The computer code of claim 21 wherein said model comprise

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a plurality of rigid bodies, each rigid body representing a portion of said molecule;

and a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies.

24. The computer code of claim 23 wherein each hinge connection comprise a connection selected from the group comprises a slide joint, a pin joint, a ball joint, and combinations thereof.

25. The computer code of claim 24 wherein q correspond to internal coordinates of one of said rigid bodies with respect to another of said rigid bodies.

26. The computer code of claim 24 wherein said internal coordinates comprise a linear displacement of said one rigid body with respect to said another rigid body.

27. The computer code of claim 24 wherein said internal coordinates comprise an angular displacement of said one rigid body with respect to said another rigid body.

28. The computer code of claim 24 wherein said internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body.

29. The computer code of claim 24 wherein M comprises a system mass matrix.

30. The computer code of claim 24 wherein f comprises a bias-free hinge torque.

31. The computer code of claim 20 wherein said implicit integrator comprises an L-stable integrator.

32. The computer code of claim 31 wherein said L-stable integrator comprises an integrator from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4 and other implicit Runge-Kutta methods.

33. A method of claim 20 wherein said implicit integrator comprises an integrator from the group comprising DASSL and other implicit multistep methods for ODE or DAE systems.

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